Dry sliding contact between fractal and statistical rough surfaces at the atomic scale

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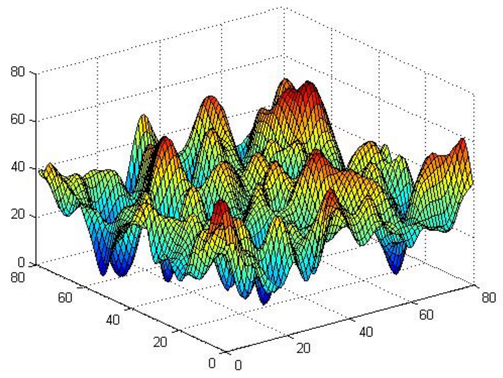
Introduction

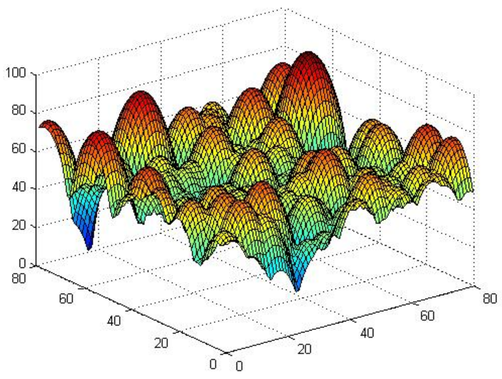
Surface roughness has a major impact on the tribology of sliding systems, from macro- to nanoscale. Because the macroscopic laws of friction break down at the atomic scale, numerical simulations, such as molecular dynamics (MD), are used to study these systems. Here we present initial results on the frictional behavior of randomly rough surfaces (in atomic scale) in dry conditions. Two different representations of surface roughness at the nanoscale are used and their effects on dry sliding contact are studied. Building on these results, we aim to study nanoscale lubricated frictional contact in future work.

Randomly rough surfaces

Two different representations of randomly rough surfaces were utilized: fractal and statistical (based on the GW model). A pair of surfaces was generated via each method.

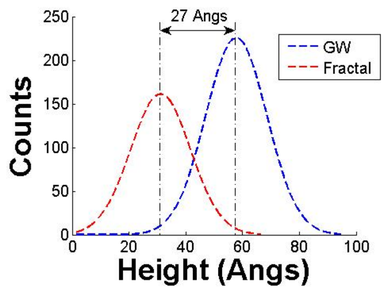


- Fractal surfaces based on Garcia and Stoll method [1]
- $\sigma = 10$ Å, $C_L = 8$ Å



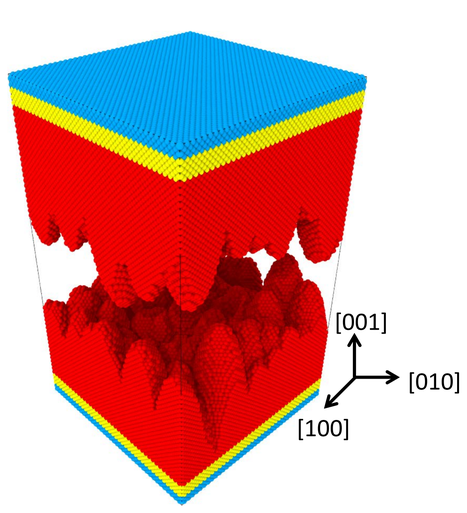
- Gaussian surfaces based on Greenwood-Williamson model [2]
- $\sigma = 10$ Å, $R = 30$ Å, $\eta = 0.01$ Å^{-2}

	GW surfaces	Fractal surfaces
σ (Å)	10.753	10.582
Skewness	0.387	0.125
Kurtosis	4.248	3.063

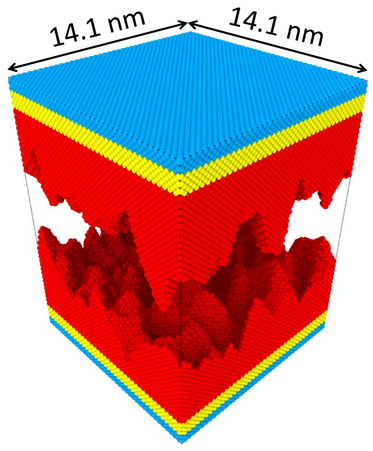


Atomic blocks

Two atomic blocks of fcc crystal structure (Nickel) were constructed using each pair of the tribo-surfaces, with a minimum thickness of $3.52\ nm$.



$\boldsymbol{I}$: System with the GW surfaces
302926 atoms



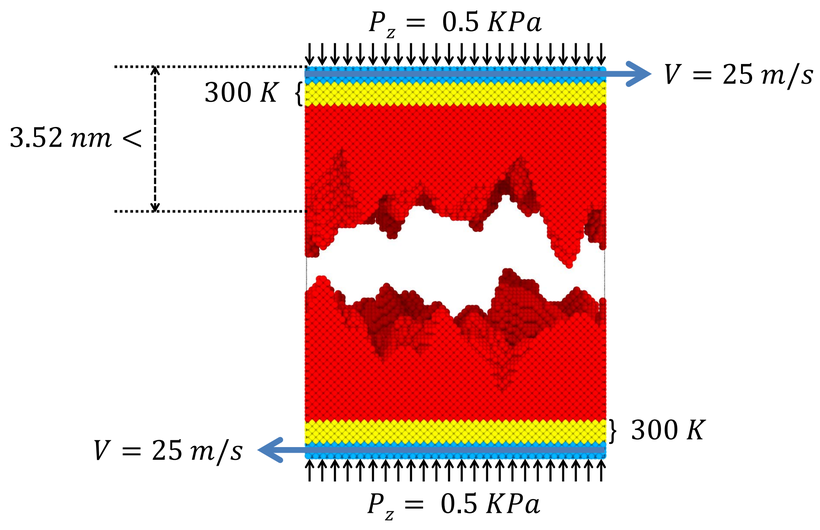
$\boldsymbol{II}$: System with the fractal surfaces
205995 atoms

Simulation setup

- Embedded Atom Model (EAM) potential for Ni [3]
- Velocity-Verlet, with an integration step size of $10\ fs$
- Periodic Boundary Conditions (PBC) in the lateral directions
- Berendsen thermostat
- Each of the two bodies was divided into three layers: rigid layer, thermostat layer, and free deformable layer.

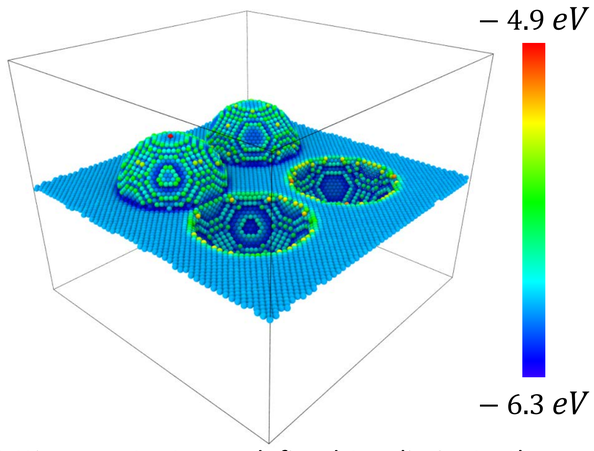
Simulation procedures

The simulations (using LAMMPS [4]) were performed in two sequential steps: compression (including equilibration) and sliding. Sliding was simulated for $3\ ns$.

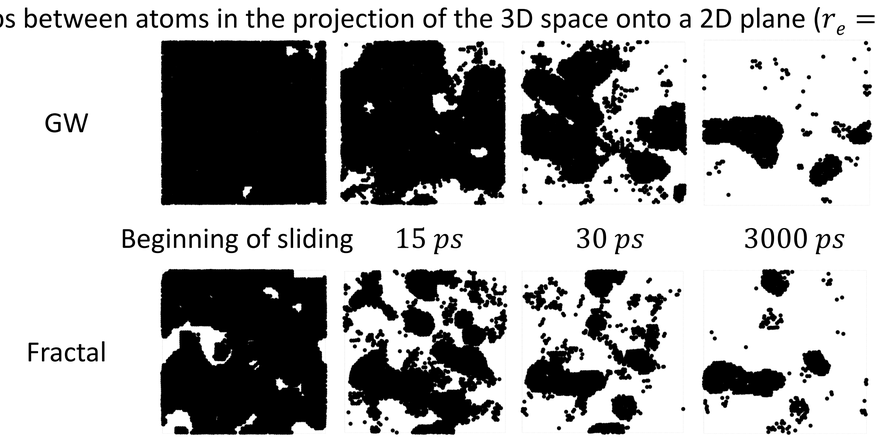


Contacting atoms and area

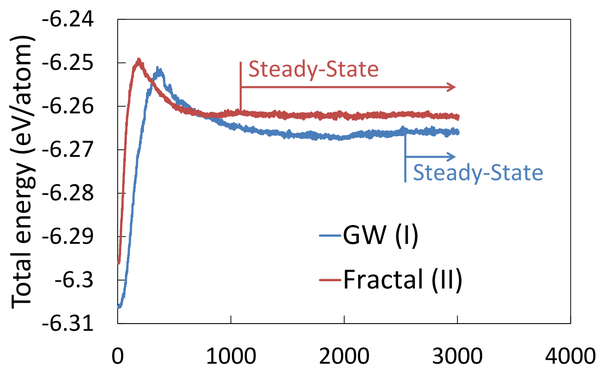
- A potential energy cutoff (PE_C) was defined to distinguish between contacted and non-contacted atoms: a system comprised of 30 Å -radius spherical asperities was created, and the minimum value of the potential energy of surface atoms ($-6.3\ eV$) was adopted as the PE_C.
- The contacting area at each desired step was estimated from the normal projection of the corresponding snapshot of non-contacted surface atoms [3].



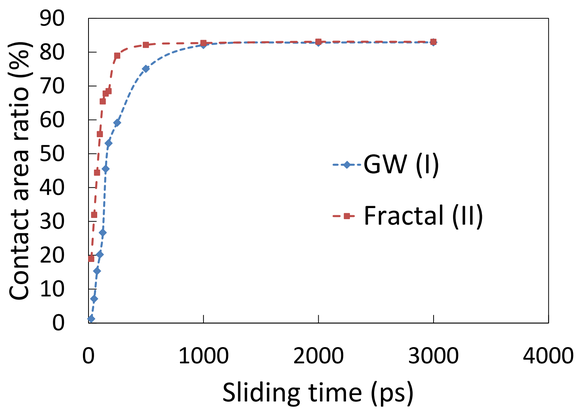
An effective radius equivalent to half of the lattice constant was defined to eliminate the gaps between atoms in the projection of the 3D space onto a 2D plane ($r_e = 1.76$ Å).



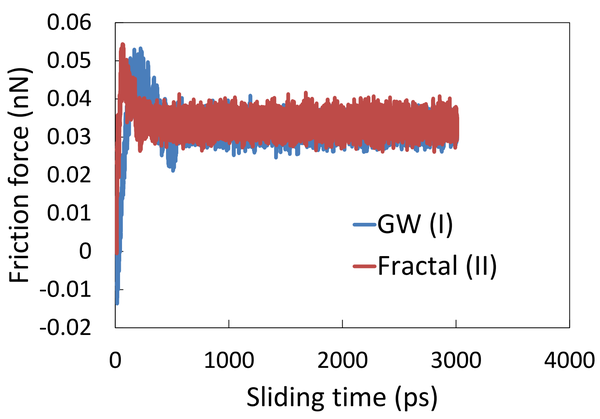
Results



Total energy of the system: The value of the total energies per atom at the end of sliding were $-6.262\ eV/atom$ and $-6.266\ eV/atom$ for the systems $\boldsymbol{I}$ and $\boldsymbol{II}$, respectively. The system $\boldsymbol{I}$ reached the steady state after $\sim 2.5\ ns$, while the system $\boldsymbol{II}$ stabilized after $\sim 1\ ns$.



Contact area ratio: The final values were similar (within $\sim 83\%$). However, the system $\boldsymbol{II}$ reached its final state faster ($\sim 0.5\ ns$) than the system $\boldsymbol{I}$ ($\sim 1\ ns$).



Friction force: Both systems showed a high friction force ($\sim 0.05\ nN$) at the beginning of the sliding corresponding to the static friction. Then, the friction force droped to a lower value ($\sim 0.03\ nN$) correspoding to the kinetic friction.

Conclusion

- Both systems show the same frictional behavior.
- The MD simulations of the systems with the fractal surfaces were faster than the systems with the corresponding GW surfaces, mainly due to ***the higher mean height of the GW surfaces***. This affected the simulations in two ways:
  1. The system with the GW surfaces needed a higher number of atoms to construct the atomic block → slower simulation during each step.
  2. This system needed more time to reach its final topography during the friction process.

Reference: **[1]** Garcia and Stoll (1984) Physical Review Letters **52**, p. 1798. **[2]** Greenwood and Williamson (1966) Proceedings of the Royal Society of London A **295**, p. 300. **[3]** Sheng et al. (2011), Physical Review B **83**, p. 134118. **[4]** Plimpton (1995) Journal of Computational Physics **117**, p. 1. **[5]** Stukowski (2010) Modelling and Simulation in Materials Science and Engineering **18**, p. 015012.